

Appendix A. Specific modifications for UPP files

A1 VRBLS3D_mod.f

After line 27

```
! Add GFS fields
      ,O3(:,:,:),O(:,:,:),O2(:,:,:) &
      ,NO(:,:,:),NO2(:,:,:),SO2(:,:,:),-
CO(:,:,:) &
      ,HCHO(:,:,:),PMTC(:,:,:),PMTF(:,:,:)

```

A2 ALLOCATEALL.f

After line 110

```
!GFS FIELD
      allocate(o3(im,jsta_21:jend_2u,lm))
      ...
      allocate(NO(im,jsta_21:jend_2u,lm))
      allocate(NO2(im,jsta_21:jend_2u,lm))
      allocate(SO2(im,jsta_21:jend_2u,lm))
      allocate(CO(im,jsta_21:jend_2u,lm))
      allocate(HCHO(im,jsta_21:jend_2u,lm))
      allocate(PMTC(im,jsta_21:jend_2u,lm))
      allocate(PMTF(im,jsta_21:jend_2u,lm))

```

A3 RQSTFLD.f

After line 1611

```
! GFS fields Chemistry Add

      DATA IFILV(510),AVBL(510),IQ(510),I
S(510),AVBLGRB2(510) &
      & /1,'SO2 ON MDL
SFCS      ',232,109,&
      & 'SO2 con-
centration ppb' / !table 141 232
      DATA IFILV(511),AVBL(511),IQ(511),I
S(511),AVBLGRB2(511) &
      & /1,'CO ON MDL
SFCS      ',148,109,&
      & 'CO concen-
tration ppb' / !table 141 148
      DATA IFILV(512),AVBL(512),IQ(512),I
S(512),AVBLGRB2(512) &
      & /1,'HCHO ON
MDL SFCS      ',166,109,&
      & 'Formal-
dehyde conc ppb' / !table 141 166
      DATA IFILV(513),AVBL(513),IQ(513),I
S(513),AVBLGRB2(513) &
      & /1,'O3 ON MDL

```

```
SFCS      ',180,109,&
      & 'Ozone conc.
ppb      '/ !table 129 180
      DATA IFILV(514),AVBL(514),IQ(514),I
S(514),AVBLGRB2(514) &
      & /1,'SURFACE O3
CONC      ',180,100,&
      & 'Ozone surf
conc ppb '/ !table 129
      DATA IFILV(515),AVBL(515),IQ(515),IS
(515),AVBLGRB2(515) &
      & /1,'PMTC ON
MDL SFCS      ',156,109,&
      & 'PM 10 conc
ug/m3      '/ !table 129 156
      DATA IFILV(516),AVBL(516),IQ(516),IS
(516),AVBLGRB2(516) &
      & /1,'PMTF ON MDL
SFCS      ',157,109, &
      & 'PM 2.5 conc
ug/m3      '/ !table 129 157
      DATA IFILV(517),AVBL(517),IQ(517),I
S(517),AVBLGRB2(517) &
      & /1,'NO ON MDL
SFCS      ',141,109,&
      & 'NO concen-
tration ppb ' / !table 141 141
      DATA IFILV(518),AVBL(518),IQ(518),I
S(518),AVBLGRB2(518) &
      & /1,'NO2 ON MDL
SFCS      ',142,109,&
      & 'NO2 con-
centration ppb' / !table 141 142

```

A4 DEALLOCATE.f

Include the following lines after line 111:

```
!GFS FIELD
      deallocate(O3)
      deallocate(NO)
      deallocate(NO2)
      deallocate(SO2)
      deallocate(CO)
      deallocate(HCHO)
      deallocate(PMTC)
      deallocate(PMTF)

```

A5 INITPOST.F

After line 48.

```

      use vrbls3d, only: t, u, uh, v, vh,
      wh, q, pmid, t, omga, pint, alpint, &
      qqr, qqs, qqi, qqg, qqni, qqnr,
      cwm, qqw, qqi, qqr, qqs, extcof55, &
      f_ice, f_rain, f_rimef, q2,
      zint, zmid, cfr, REF_10CM, &
      o3, co, no, no2, so2, pmtf, pmtc, hcho

```

After line 341. (Because WRF-chem model has gas concentrations in ppm a conversion to ppb is made multiplying by 1000 only gas chemical variables).

```

      print*, 'finish reading mixing ratio'
! For Particulate Matter (Coarse) PM10
      VarName='PM10'
      call getVariable(fileName, DateStr, -
DataHandle, VarName, DUM3D, &
      IM+1, 1, JM+1, LM+1, IM, JS, JE, LM)
      do l = 1, lm
        do j = jsta_21, jend_2u
          do i = 1, im
            PMTC( i, j, l ) = dum3d ( i,
j, l )
          end do
        end do
      end do
! For Particulate Matter (Fine) PM2.5
      VarName='PM2_5_DRY'
      call getVariable(fileName, DateStr, -
DataHandle, VarName, DUM3D, &
      IM+1, 1, JM+1, LM+1, IM, JS, JE, LM)
      do l = 1, lm
        do j = jsta_21, jend_2u
          do i = 1, im
            PMTF( i, j, l ) = dum3d ( i,
j, l )
          end do
        end do
      end do
      print*, 'finish reading PM10 and PM2.5
concentrations'
! For Ozone O3
      VarName='o3'
      call getVariable(fileName, DateStr, Da-
taHandle, VarName, DUM3D, &
      IM+1, 1, JM+1, LM+1, IM, JS, JE, LM)
      do l = 1, lm

```

```

        do j = jsta_21, jend_2u
          do i = 1, im
            O3( i, j, l ) = dum3d ( i, j,
1 ) * 1000.
          end do
        end do
      end do
! For Nitrogen Oxides NO
      VarName='no'
      call getVariable(fileName, DateStr, Da-
taHandle, VarName, DUM3D, &
      IM+1, 1, JM+1, LM+1, IM, JS, JE, LM)
      do l = 1, lm
        do j = jsta_21, jend_2u
          do i = 1, im
            NO( i, j, l ) = dum3d ( i, j,
1 ) * 1000.
          end do
        end do
      end do
! For Nitrogen Dioxide NO2
      VarName='no2'
      call getVariable(fileName, DateStr, Da-
taHandle, VarName, DUM3D, &
      IM+1, 1, JM+1, LM+1, IM, JS, JE, LM)
      do l = 1, lm
        do j = jsta_21, jend_2u
          do i = 1, im
            NO2( i, j, l ) = dum3d ( i, j,
1 ) * 1000.
          end do
        end do
      end do
! For Sulfur Dioxide SO2
      VarName='so2'
      call getVariable(fileName, DateStr, Da-
taHandle, VarName, DUM3D, &
      IM+1, 1, JM+1, LM+1, IM, JS, JE, LM)
      do l = 1, lm
        do j = jsta_21, jend_2u
          do i = 1, im
            SO2( i, j, l ) = dum3d ( i, j,
1 ) * 1000.
          end do
        end do
      end do
! For Carbon Monoxide CO
      VarName='co'

```

```

call getVariable(fileName,DateStr,DataHandle,VarName,DUM3D,
    &
    IM+1,1,JM+1,LM+1,IM,JS,JE,LM)
do l = 1, lm
do j = jsta_2l, jend_2u
do i = 1, im
CO( i, j, l ) = dum3d ( i, j, JM)
l )*1000.
end do
end do
end do
! For Formaldehyde HCHO
VarName='hcho'
call getVariable(fileName,DateStr,DataHandle,VarName,DUM3D,
    &
    IM+1,1,JM+1,LM+1,IM,JS,JE,LM)
do l = 1, lm
do j = jsta_2l, jend_2u
do i = 1, im
HCHO( i, j, l ) = dum3d ( i, j, l )*1000.
end do
end do
end do
print*, '*** Finish reading gas chemical concentrations'

A6 MDLFLD.f
After line 82
use vrbls3d, only: zmid, t, pmid, q, cwm, f_ice, f_rain, f_rimef, qqw, qqi,&
    qqr, qqs, cfr, dbz, dbzr, dbzi, dbzc, qqw, nlice, nrain, qgg, zint, qqni,&
    qqnr, uh, vh, mcvg, omga, wh, q2, ttnd, rswtt, rlwtt, train, tcucn,&
    o3, rhomid, dpres, el_pbl, pint, icing_gfip, icing_gfis, REF_10CM,&
    co,no,no2,so2,pmtf,pmtc,hcho

After line 2049
! Nitrogen Oxide (NO) ON MDL SURFACES.
IF (IGET(517).GT.0) THEN
IF (LVLS(L,IGET(517)).GT.0) THEN
LL=LM-L+1
ID(1:25) = 0
ID(2)=141
!$omp parallel do private(i,j)
DO J=JSTA,JEND
DO I=1,IM
GRID1(I,J)=NO(I,J,LL)
ENDDO
ENDDO
if(grib=="grib1") then
CALL GRIBIT(IGET(517),L,GRID1,IM,-JM)
else if(grib=="grib2") then
cfld=cfld+1
fld_info(cfld)%i-
fld=IAVBLFLD(IGET(517))
fld_info(cfld)%lvl=LVLXSM-L(L,IGET(517))
!$omp parallel do private(i,j,jj)
do j=1,jend-jsta+1
jj = jsta+j-1
do i=1,im
datapd(i,j,cfld) =
GRID1(i,jj)
enddo
enddo
endif
ENDIF
ENDIF
! Nitrogen Dioxide (NO2) ON MDL SURFACES.
IF (IGET(518).GT.0) THEN
IF (LVLS(L,IGET(518)).GT.0) THEN
LL=LM-L+1
ID(1:25) = 0
ID(2)=141
!$omp parallel do private(i,j)
DO J=JSTA,JEND
DO I=1,IM
GRID1(I,J)=NO2(I,J,LL)
ENDDO
ENDDO
if(grib=="grib1") then
CALL GRIBIT(IGET(518),L,GRID1,IM,-JM)
else if(grib=="grib2") then
cfld=cfld+1
fld_info(cfld)%i-
fld=IAVBLFLD(IGET(518))
fld_info(cfld)%lvl=LVLXSM-L(L,IGET(518))
!$omp parallel do private(i,j,jj)
do j=1,jend-jsta+1
jj = jsta+j-1

```

```

                do i=1,im
                    datapd(i,j,cfld) =
GRID1(i,jj)
                enddo
            enddo
        endif

        ENDIF
    ENDIF
!
    Sulfur Dioxide (SO2) ON MDL  JM)
SURFACES.
        IF (IGET(510).GT.0) THEN
        IF (LVLS(L,IGET(510)).GT.0) THEN
            LL=LM-L+1
            ID(1:25) = 0
            ID(2)=141
!$omp parallel do private(i,j)
            DO J=JSTA,JEND
                DO I=1,IM
                    GRID1(I,J)=SO2(I,J,LL)
                ENDDO
            ENDDO
                if(grib=="grib1") then
                CALL GRIBIT(IGET(510),L,GRID1,IM,-
JM)
                else if(grib=="grib2" )then
                    cfld=cfld+1
                    fld_info(cfld)%i-
fld=IAVBLFLD(IGET(510))
                    fld_info(cfld)%lvl=LVLSXM-
L(L,IGET(510))
!$omp parallel do private(i,j,jj)
                    do j=1,jend-jsta+1
                        jj = jsta+j-1
                        do i=1,im
                            datapd(i,j,cfld) =
GRID1(i,jj)
                        enddo
                    enddo
                endif
            ENDIF
        ENDIF
!
        Formaldehyde (HCHO) ON MDL SUR-
FACES.
        IF (IGET(512).GT.0) THEN
        IF (LVLS(L,IGET(512)).GT.0) THEN
            LL=LM-L+1
            ID(1:25) = 0
            ID(2)=141
!$omp parallel do private(i,j)
            DO J=JSTA,JEND
                DO I=1,IM
                    GRID1(I,J)=HCHO(I,J,LL)
                ENDDO
            ENDDO
                if(grib=="grib1") then
                CALL GRIBIT(IGET(512),L,GRID1,IM,-
JM)
                else if(grib=="grib2" )then
                    cfld=cfld+1
                    fld_info(cfld)%i-
fld=IAVBLFLD(IGET(512))
                    fld_info(cfld)%lvl=LVLSXM-
L(L,IGET(512))

```

```

!$omp parallel do private(i,j,jj)
    do j=1,jend-jsta+1
        jj = jsta+j-1
        do i=1,im
            datapd(i,j,cfld) =
GRID1(i,jj)
                enddo
            enddo
        endif
    endif
ENDIF
ENDIF
!
    OZONE (O3) ON MDL SURFACES.
    IF (IGET(513).GT.0) THEN
    IF (LVLS(L,IGET(513)).GT.0) THEN
        LL=LM-L+1
        ID(1:25) = 0
        ID(2)=129
!$omp parallel do private(i,j)
        DO J=JSTA,JEND
            DO I=1,IM
                GRID1(I,J)=O3(I,J,LL)
            ENDDO
        ENDDO
        if(grib=="grib1") then
            CALL GRIBIT(IGET(513),L,GRID1,IM,-
JM)
        else if(grib=="grib2" )then
            cfld=cfld+1
            fld_info(cfld)%i-
fld=IAVBLFLD(IGET(513))
            fld_info(cfld)%lvl=LVLSXM-
L(L,IGET(513))
!$omp parallel do private(i,j,jj)
            do j=1,jend-jsta+1
                jj = jsta+j-1
                do i=1,im
                    datapd(i,j,cfld) =
GRID1(i,jj)
                        enddo
                enddo
            endif
        endif
    endif
ENDIF
ENDIF
!
    PMTC (PM10) ON MDL SURFACES.
    IF (IGET(515).GT.0) THEN
    IF (LVLS(L,IGET(515)).GT.0) THEN
        LL=LM-L+1
        ID(1:25) = 0

```

```

        ID(2)=129
!$omp parallel do private(i,j)
        DO J=JSTA,JEND
            DO I=1,IM
                GRID1(I,J)= PMTC(I,J,LL)
            ENDDO
        ENDDO
        if(grib=="grib1") then
            CALL GRIBIT(IGET(515),L,GRID1,IM,-
JM)
        else if(grib=="grib2" )then
            cfld=cfld+1
            fld_info(cfld)%i-
fld=IAVBLFLD(IGET(515))
            fld_info(cfld)%lvl=LVLSXM-
L(L,IGET(515))
!$omp parallel do private(i,j,jj)
            do j=1,jend-jsta+1
                jj = jsta+j-1
                do i=1,im
                    datapd(i,j,cfld) =
GRID1(i,jj)
                        enddo
                enddo
            endif
        endif
    endif
ENDIF
ENDIF
!
    PMTF (PM2.5) ON MDL SURFACES.
    IF (IGET(516).GT.0) THEN
    IF (LVLS(L,IGET(516)).GT.0) THEN
        LL=LM-L+1
        ID(1:25) = 0
        ID(2)=129
!$omp parallel do private(i,j)
        DO J=JSTA,JEND
            DO I=1,IM
                GRID1(I,J)= PMTF(I,J,LL)
            ENDDO
        ENDDO
        if(grib=="grib1") then
            CALL GRIBIT(IGET(516),L,GRID1,IM,-
JM)
        else if(grib=="grib2" )then
            cfld=cfld+1
            fld_info(cfld)%i-
fld=IAVBLFLD(IGET(516))
            fld_info(cfld)%lvl=LVLSXM-
L(L,IGET(516))

```

```

!$omp parallel do private(i,j,jj)
    do j=1,jend-jsta+1
        jj = jsta+j-1
        do i=1,im
            datapd(i,j,cfld) =
GRID1(i,jj)
                enddo
            enddo
        endif
    ENDIF
ENDIF
!
! ---- ADD GOCART FIELDS

A7 wrf cntrl.parm
-
Additional lines to be add.
    (O3 ON MDL SFCS      ) SCAL=( 4.0)
    L=(10000 00000 00000 00000 00000 00000
00000 00000 00000 00000 00000 00000 00000)
    (NO ON MDL SFCS      ) SCAL=( 4.0)
    L=(10000 00000 00000 00000 00000 00000
00000 00000 00000 00000 00000 00000 00000)
    (NO2 ON MDL SFCS      ) SCAL=( 4.0)

    L=(10000 00000 00000 00000 00000 00000
00000 00000 00000 00000 00000 00000 00000)
    (SO2 ON MDL SFCS      ) SCAL=( 4.0)
    L=(10000 00000 00000 00000 00000 00000
00000 00000 00000 00000 00000 00000 00000)
    (CO ON MDL SFCS      ) SCAL=( 4.0)
    L=(10000 00000 00000 00000 00000 00000
00000 00000 00000 00000 00000 00000 00000)
    (HCHO ON MDL SFCS     ) SCAL=( 4.0)
    L=(10000 00000 00000 00000 00000 00000
00000 00000 00000 00000 00000 00000 00000)
    (SURFACE O3 CONC      ) SCAL=( 4.0)
    L=(00000 00000 00000 00000 00000 00000
00000 00000 00000 00000 00000 00000 00000)
    (PMTc ON MDL SFCS     ) SCAL=( 4.0)
    L=(10000 00000 00000 00000 00000 00000
00000 00000 00000 00000 00000 00000 00000)
    (PMTF ON MDL SFCS     ) SCAL=( 4.0)
    L=(10000 00000 00000 00000 00000 00000
00000 00000 00000 00000 00000 00000 00000)

```